INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XXI, 1127–1129 (1982)

Author Index to Volume XXI

Abdul-Ahad, P. G. and Webb, G. A.: Interpretation of the Antitumor Activity of Some Diacridines, 945
— and —: Quantitative Structure Activity Relationships for Some Antitumor Platinum(II) Complexes, 1105
Adams, B. G., Čížek, J., and Paldus, J.: Representation Theory of *so* (4,2) for the Perturbation Treatment Hydrogenic-Type Hamiltonians by Algebraic Method, 153
Almlöf, J.: See Grelland, H. S.
Au, C. K.: Perturbation Theory via the Ricatti Equation, 179
Avery, J., Ørmen, P.-J., and Chatterjee, I.: Transferable Integrals in a Deformation Density Approach to Crystal Calculations. I. Crystal Harmonics and Their Properties, 515
Avron, J. E.: Bender–Wu Formulas and Classical Trajectories: Higher Dimensions and Degeneracies, 119

Bačić, Z., and Simons, J.: Complex Coordinate Rotation Calculation of Branching Ratios, 727
Balasubramanian, K.: Symmetry Groups of Chemical Graphs, 411
—: Spectra of Chemical Trees, 581
Banerjee, M. and Bhattacharyya, S. P.: Scaled One-Electron Hamiltonian Model for open-Shell LCAO–MO–SCF Calculations: Comparison with the Restructed Open-Shell Method of Roothaan, 905
Bender, C. M.: Perturbation Theory in Large Order for Some Elementary Systems, 93
Bhattacharjee, S.: See De, B. R.
Bhattacharyya, K.: Feenberg Scaling and Higher-Order Invariants in Rayleigh–Schrödinger Perturbation Theory, 857
Bhattacharyya, S. P.: Semiempirical Molecular Orbital Calculations on Octahedral Aquo Complexes of Transition Metal Ions: σ-Donor Ability of Water, 851
—: See Banerjee, M.
Birner, P. and Hofmann, H.-J.: Critical Examination of Approximate LCAO MO Methods. I. Reasons for the Failure of the CNDO and INDO Methods in Theoretical Conformational Analysis of Conjugated Compounds, 833
Biskupič, S. and Kvasnička, V.: Construction of an Effective Hamiltonian for Open-Shell Molecular Systems, 633
Black, R. J. and Stedman, G. E.: Diagram Approach to Group Algebraic Methods, 823
Brändas, E. J., Combs, L. L., and Correia, N. S.: Size Consistency Corrections for Configurations Interaction Calculations, 259

Calais, J.-L.: Is Quantum Chemistry Concerned with Materials Science?, 231
—: See Löwdin, P.-O.
Castro, E. A.: See Fernández, F. M.
Chatterjee, I.: See Avery, J.
Cheney, B. V.: Structural Factors Affecting Aryl Hydrocarbon Hydroxylase Induction by Dibenzo-*p*-dioxins and Dibenzofurans, 445
Čížek, J.: See Adams, B. G.
—: See Pellegatti, A.
— and Vrscay, E. R.: Large Order Perturbation Theory in the Context of Atomic and Molecular Physics—Interdisciplinary Aspects, 27
Colditz, R.: See Gustav, K.
Combs, L. L.: See Brändas, E. J.
—: See Dunne, L. J.
Corrêa De Mello, P., Hehenberger, M., and Zerner, M. C.: Converging SCF Calculations on Excited States, 251
Correia, N. S.: See Brändas, E. J.
Csavinszky, P.: Theory of the Electron Distribution in Compressed Atoms at High Temperature, 899
Csizmadia, I. G.: See Daudel, R.
—: See Poirier, R. A.

Damburg, R. and Propin, R.: Double Wells, 191
Das, M. P.: Calculation of Relaxed Orbital Binding Energies in Atoms: Zinc and Cadmium, 845
Daudel, R.: See Poirier, R. A.
—, Poirier, R. A., and Csizmadia, I. G.: Uniform Quality Gaussian Basis Sets for Molecular Calculations. V. Property Optimization: A Study on H_2O, 699
Day, R. S. and Ladik, J.: Cluster CPA Calculations for Infinite and Half-Infinite Chains and Applications to Coupled Polymer Chains, 917
De, B. R., Bhattacharjee, S., and Sannigrahi, A. B.: CNDO/2 and INDO Studies of Structure and Relative Stability of a Series of H*AB*-H*BA* Systems of Mixed First- and Second-Row Composition, 665
Del Re, G.: See Mezey, P. G.
Dunne, L. J., and Combs, L.: Towards a Molecular Theory of Phase Transitions in Fatty Acid Monolayers, 239

Easa, S. I. and Yousif, F. N.: Long-Range Interaction Coefficients between H, He^+, He, and Li^+, 1117
El-Basil, S.: Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. I. Simple Catacondensed Systems, 771
El-Basil, S.: Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. II. Benzenoid Systems Having Four to Seven Fused Benzene Rings: "Pseudodegenerate" States, 779
El-Basil, S.: Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. III. Nonalternate and Nonbenzenoid Hydrocarbons, 793
Essén, H.: Periodic Table of the Elements and the Thomas–Fermi Atom, 717

Fedyanin, V. K. and Yakushevich, L. V.: Particlelike Excitations in the Polypeptide Chain Model, 1019
Fernández, F. M. and Castro, E. A.: Trivial Off-Diagonal Hellmann–Feynman Formulas, 671
— and —: Hypervirial Extension for Energies of Parameter-Dependent Systems, 673
— and —: Virial Theorem and Boundary Conditions for Approximate Wave Functions, 741
— and —: Hypervirial Analysis of Enclosed Quantum Mechanical Systems. IV. Further Comments, 875
— and —: Some Comments about Tensor Virial Theorem and Linear Transformations, 1097

© 1982 John Wiley & Sons, Inc.

Gallup, G. A.: Transformation of Spin Projected Slater Determinants under Orbital Permutation, 1057
Graffi, S.: Meaning of the Perturbation Theory for a Class of Multiple-Well Anharmonic Oscillators, 195
Goscinski, O.: Some Properties of Reduced Density Matrices, Correlated and Uncorrelated, for Pure and Mixed States, 269
—: See Löwdin, P.-O.
—: See Weiner, B.
Grelland, H. S. and Almlöf, J.: Reduced Local Energy as a Criterion for the Accuracy of Approximate Hartree-Fock Wave Functions Application to H_2O and CH_4, 885
Groenendael, A. V.: See Smet, F.
Gustav, K. and Colditz, R.: Potential Adaption: Use of Polynomials as Anharmonic Oscillator Potentials, 1091

Hamano, H.: Variational Solutions of a First-Order Perturbation Equation, 611
Harrell, E. M., II: Estimating Tunneling Phenomena, 199
Hashimoto, K.: Charge and Spin Correlation Structures of Conjugated π Systems: Analysis of Full CI Wave Functions of the PPP Hamiltonian, 861
Hayns, M. R.: Relevance of the Techniques of Quantum Chemistry in Materials Science and Related Areas, 217
Hehenberger, M.: See Corrêa De Mello, P.
Helgaker, T. U.: Simple Derivation of the Potential Energy Gradient for an Arbitrary Electronic Wave Function (*Letter to the Editor*), 939
Hofmann, H.-J.: See Birner, P.
Hunter, G., and Tai, C. C.: Variational Marginal Amplitudes, 1041

Iijima, T.: See Sasaki, Y.

Jolly, P., Sane, K. V., Saxena, R. P., and Srivastava, P. K.: Some Remarks on the Use of Rational Functions as Variational Functions, 1051
Jones, H. W.: Evaluation of Two-Center Overlap and Coulomb Integrals Derived from Slater-Type Orbitals, 1079

Katović, V.: See Randić, M.
Khuri, N. N.: Failure of Strong Asymptotic Conditions in Four-Dimensional Field Theories, 173
Kimura, M.: See Sasaki, Y.
Konaka, S.: See Sasaki, Y.
Krechl, J. and Kuthan, J.: Molecular Orbital Study on the Active Center of Lactate Dehydrogenase, 1029
Kryachko, E. S.: Matrix Analysis of *N*-Representability Necessary Conditions, 1123
Kuthan, J.: See Krechl, J.
Kvasnička, V.: Permutation-Group Classification and Description of the Feynman-Goldstone Diagrams, 1003
—: See Biskupič, S.

Ladik, J.: See Day, R. S.
—: See Mezey, P. G.
Laidlaw, W.: See Trsic, M.
László, I.: CNDO/2 Calculations of Relaxation and Reconstruction of Diamond and Silicon [111] Surfaces, 813
Lee, K. F.: See Malinowski, P.
Levy, M. and Perdew, J. P.: In Defense of the Hohenberg-Kohn Theorem and Density Functional Theory (*Letter to the Editor*), 511
Linder, B.: See Malinowski, P.
Lochmann, R. and Weller, Th.: Calculation of Periodic Molecular Systems with Perturbed Periodicity within the PCILO Framework. I. Method, 711
Löwdin, P.-O.: Partitioning Technique, Perturbation Theory, and Rational Approximations, 69
—: On the Axioms of Quantum Theory Formulated as a Trace Algebra, 275
—, Calais, J.-L., and Goscinski, O.: Preface (Proceedings of the Tarfala Workshop), 215
—, Calais, J.-L., and Goscinski, O.: Editorial: Density Functional Theory, 357
—, and Öhrn, Y.: Introduction (Proceedings of the International Workshop on Perturbation Theory at Large Order), 1
Ludeña, E. B. and Mujica, V.: Virial Fragments and the Hohenberg-Kohn Functional, 927
Lunell, S.: By Arthur W. Adamson (*Book Review*), 941

Malinowski, P., Tanner, A. C., Lee, K. F., and Linder, B.: Calculation in k Space of Integrals Arising in the Theory of van der Waals Force, 753
Malykhanov, Yu. B.: Variational-Perturbation Theory in the LCAO-MO Method for Closed-Shell Molecules, 399
Mezey, P. G.: See Poirier, R. A.
—, Del Re, G., Otto, P., Suhai, S., and Ladik, J.: Charge Transfer and Induced Polarization in Model Peptide–Ion Complexes, 677
Moskowitz, J. W.: See Snyder, L. C.
Mujica, V.: See Ludeña, E. B.
Müller, J.: Configuration Interaction Calculations of the Valence and the Inner Valence Levels of the CS Molecule, 465

Öhrn, Y.: See Löwdin, P. O.
Oriade, J.: Electronic Structure of Beryllium, 359
Ørmen, P. J.: See Avery, J.
Otto, P.: See Mezey, P. G.

Paldus, J.: See Adams, B. G.
—: See Pellegatti, A.
Pellegatti, A., Čížek, J., and Paldus, J.: Numerical Estimates of the Convergence of the Rayleigh–Schrodinger Perturbation Expansions for the Energy Levels of Various Models of the Benzene Molecule, 147
Perdew, J. P.: See Levy, M.
Poirier, R. A.: See Daudel, R.
—, Daudel, R., Mezey, P. G., and Csizmadia, I. G.: *Ab initio* Calculations on Sulfur Containing Compounds. I. Uniform Quality Basis Sets for Sulfur: Total Energies and Geometries of H_2S, 799
Propin, R.: See Damburg, R.

Randić, M. and Katović, V.: Symmetry Properties of Chemical Graphs. IV. Rearrangement of Tetragonal-Pyramidal Complexes, 647
Reinhardt, W. P.: Padé Summations for the Real and Imaginary Parts of Atomic Stark Eigenvalues, 133

Sakamoto, K.: See Terasaka, T.
Sane, K. V.: See Jolly, P.
Sannigrahi, A. B.: See De, B. R.
Sasaki, Y., Konaka, S., Iijima, T., and Kimura, M.: Small-Angle Electron Scattering and Electron Density in Carbon Dioxide, 475
Saxena, R. P.: See Jolly, P.
Silverstone, H. J.: Unified Derivation of the Perturbation

Series for the Real and Imaginary Parts of the Energy of Hydrogen in the Stark Effect and of the Negatively Anharmonic Oscillator, 125
Simas, A. M., Thakkar, A. J., and Smith, V. H., Jr.: Momenturm Space Properties of Various Orbital Basis Sets Used in Quantum Chemical Calculations, 419
Simon, B.: Large Orders and Summability of Eigenvalue Perturbation Theory: A Mathematical Overview, 3
Simons, J.: See Bačić, Z.
Skancke, A. and Thomson, C.: *Ab initio* Calculations of the Electronic Structures of Dimethylnitrosamine (DMN) and Its Metabolite Hydroxydimethylnitrosamine (HDMN): A Possible Intermediate in Carcinogenesis by DMN, 431
Smet, F. and Groenendael, A. V.: Equation Matricielle de Hartree–Fock Permettant de Determiner la n^{ieme} Harmonique, 1061
Smith, V. H., Jr.: See Simas, A. M.
Snyder, L. C., Wasserman, Z. R., and Moskowitz, J. W.: Stability and Bonding of Disilyne and Its Isomers: A Generalized Valence Bond-Effective Potential Study, 565
Srivastava, P. K.: See Jolly, P.
Stedman, G. E.: See Black, R. J.
Stolarczyk, L. Z.: Molecular Tight-Binding Method. I. Many-Electron Method for Hole Bands of Molecular Crystals, 967
Stolarczyk, L. Z.: Molecular Tight-Binding Method. II. One- and Many-Electron Method for Excess Electron Bands of Molecular Crystals, 993
Suhai, S.: See Mezey, P. G.
Swenson, R. J.: Comment on Hypervirial Relations for Bounded Systems (*Letter to the Editor*), 937

Tai, C. C.: See Hunter, G.
Tanner, A. C.: See Malinowski, P.
Terasaka, T. and Sakamoto, K.: Note on Calculations by Hypervirial Relations and Sufficient Conditions for These Relations: Box Potential and Harmonic Oscillator Models, 543
Thakkar, A. J.: See Simas, A. M.
Thomson, C.: See Skancke, A.
Trsic, M. and Laidlaw, W. G.: *Ab initio* Hartree–Fock–Slater Calculation of Tetrathiafulvalene (TTF) and the TTF^{1+} and TTF^{2+} Ions, 557

Vrscay, E. R.: See Čížek, J.

Wasserman, Z. R.: See Snyder, L. C.
Webb, G. A.: See Abdul-Ahad, P. G.
Weiner, B.: General Linear Group Approach to Bivariational Problems, 591
— and Goscinski, O.: Superoperator Approach to Propagator Approximations, 369
Weinhold, F.: See Wesenberg, G.
Weller, Th.: See Lochmann, R.
Wesenberg, G., and Weinhold, F.: Coupling of Internal Rotations in Propanelike Molecules, 487
Westhaus, P.: Connections between Perturbation Theory and the Van Vleck Transformation: Illustrative Calculation on the Perturbed Harmonic Oscillator, 617
Wu, T. T.: Large-Order Perturbation Theory, 105

Yakushevich, L. V.: See Fedyanin, V. K.
Yousif, F. N.: See Easa, S. I.

Zerner, M. C.: See Corrêa De Mello, P.

International Journal of Quantum Chemistry
Information for Contributors

1. Manuscripts should be submitted to: Professor P.-O. Löwdin, Quantum Chemistry Group, University of Uppsala, Box 513. S-751 20, Uppsala 1, Sweden.

   All other correspondence should be addressed to: Journals Department, John Wiley & Sons, Inc., 605 Third Avenue, New York, New York 10158, U.S.A.
2. It is the preference of the Editors that papers be published in the English language. However, if the author desires that his paper be published in French or German, it is necessary that a particularly complete and comprehensive synopsis be furnished in English.
3. Manuscripts should be submitted in triplicate (one *original*, two carbon copies), typed *double spaced* throughout and on one side of each sheet only, on a *heavy* grade paper with margins of at least 2.5 cm on all sides. With the advent of the U.S. Copyright Law effective January 1978, the transfer of copyright from author to publisher, heretofore implicit in the submission of a manuscript, must now be clearly stated in writing to enable the publisher to assure maximum dissemination of the author's work. A copy of the transfer of copyright agreement to be used for the *International Journal of Quantum Chemistry* appears in this issue. (Additional copies are available from the Editor.) A copy of that agreement, executed and signed by the author, is now required with each manuscript submission. (If the article is a "work made for hire," the agreement must be signed by the employer.)
4. A short synopsis (maximum length 200 words) is required. The synopsis should be a summary of the entire paper, not the conclusions alone. If the paper is written in French or German, a synopsis in English should also be prepared. The paper should be reasonably subdivided into sections and, if necessary, subsections.
5. A list of five key words or phrases for indexing must accompany each submission.
6. Authors are cautioned to type—wherever possible—all mathematical and chemical symbols, equations, and formulas. If these must be handwritten, please print clearly and leave ample space above and below for printer's marks; please use only ink. All Greek or unusual symbols should be identified in the margin the first time they are used. Please distinguish in the margins of the manuscript between capital and small letters of the alphabet wherever confusion may arise (e.g., k, K, κ). Please underline with a wavy line all vector quantities. Use fractional exponents to avoid root signs.

   The nomenclature sponsored by the International Union of Pure and Applied Chemistry is requested for chemical compounds. Unit abbreviations should follow the practices of the American Institute of Physics. Chemical bonds should be correctly placed, and double bonds clearly indicated. Valence is to be indicated by superscript plus and minus signs.
7. The references should be numbered consecutively in the order of their appearance and should be complete, including authors' initials and—for unpublished lectures or symposia—the title of the paper, the date, and the name of the sponsoring society. Please compile references on a separate sheet at the end of the manuscript. Abbreviations of journal titles should conform to the *Bibliographic Guide for Editors & Authors* published by the American Chemical Society.

   References should be limited to literature citations. Explanatory or supplementary material should be treated either as footnotes to text or appendices.
8. All tables *must* be original typescript or in a form suitable for photographic reproduction (see paragraph 10). Each table should be supplied on a separate sheet (not interspersed with text). Please supply numbers and titles for all tables. All table columns should have an explanatory heading.
9. Please supply legends for all figures and compile these on a separate sheet.
10. It is particularly important that all figures be submitted in a form suitable for reproduction. Good glossy photographs are required for halftone reproductions. For line drawings (graph, etc.), the figures must be drawn clearly with India ink on heavy white paper, Bristol board, drawing linen, or coordinate paper with a very light blue background. The India ink lettering of graphs must be large, clear, and "open" so that letters and numbers do not fill in when reduced for publication. Artwork is generally reduced so that the type in the figures is about 2.5 mm high. It is the usual practice to submit drawings that are twice the size of the final reproduction; the maximum final size of figures for this journal is 12 × 19 cm. If in doubt about the preparation of illustrations suitable for reproduction, please consult the publisher at the address given in paragraph 1.

    It is the author's responsibility to obtain written permission to reproduce material which has appeared in another publication. A copy of the approved permission request should be forwarded to the Editor on acceptance of the manuscript.

11. Senior authors will receiver 50 reprints of their articles without charge. Additional reprints can be ordered and purchased by filling out the form attached to the proof.
12. The publisher will do everything possible to ensure prompt publication. It will therefore be appreciated if manuscripts and illustrations conform from the outset to the style of the journal. Contributors should use the *Style Manual* of the American Institute of Physics; papers will otherwise have to be returned to the author for revision.

    Corrected proofs must be sent back to the publisher within two days to avoid the risk of the author's contribution having to be held over to a later issue.

International Journal of

Quantum Chemistry

Volume XXI, 1982

HONORARY EDITORIAL BOARD

Robert S. Mulliken
Chicago, Illinois

Gerhard Herzberg
Ottawa, Canada

EDITORIAL OFFICE

Editor-in-Chief:

Per-Olov Löwdin
Uppsala, Sweden and Gainesville, Florida

Editors:

Jean-Louis Calais
Uppsala, Sweden

Yngve Öhrn
Gainesville, Florida

Associate Editors:

Osvaldo Goscinski
Uppsala, Sweden

John R. Sabin
Gainesville, Florida

Editorial Board:

R. Daudel
Paris, France

K. Fukui
Kyoto, Japan

J. O. Hirschfelder
Madison, Wisconsin

L. Jansen
Geneva, Switzerland

M. Kotani
Tokyo, Japan

R. McWeeny
Sheffield, England

R. G. Parr
Chapel Hill, North Carolina

R. Pauncz
Haifa, Israel

J. A. Pople
Pittsburgh, Pennsylvania

B. Pullman
Paris, France

C. C. J. Roothaan
Chicago, Illinois

H. Shull
Bloomington, Indiana

an Interscience® Publication, published by **JOHN WILEY & SONS**

Advisory Editorial Board

J.-M. André
Namur, Belgium

A. v. d. Avoird
Nijmegen, The Netherlands

C.-J. Ballhausen
Copenhagen, Denmark

S. Basu
Calcutta, India

A. Dalgarno
Cambridge, MA

E. Davidson
Seattle, WA

I. Fischer-Hjalmars
Stockholm, Sweden

R. Flannery
Atlanta, GA

A. A. Frost
Sedona, AR

F. A. Gianturco
Bari, Italy

G. G. Hall
Nottingham, England

F. E. Harris
Salt Lake City, UT

A. C. Hurley
Clayton, Australia

K.-H. Hsu
Peking, China

J. I'Haya
Tokyo, Japan

J. J. Kaufman
Baltimore, MD

W. Kolos
Warsaw, Poland

J. Koutecky
Berlin, West Germany

W. Kutzelnigg
Bochum, West Germany

J. Ladik
Erlangen, West Germany

W. Lester
Berkeley, CA

J. Linderberg
Aarhus, Denmark

R. Manne
Bergen, Norway

F. A. Matsen
Austin, TX

H. V. McIntosh
Puebla, Mexico

D. Micha
Gainesville, FL

W. Miller
Berkeley, CA

K. Morokuma
Okazaki, Japan

K. Ohno
Sapporo, Japan

A. Ovchinnikov
Moscow, Russia

J. Paldus
Waterloo, Canada

S. Peyerimhoff
Bonn, West Germany

H. Preuss
Stuttgart, West Germany

I. Prigogine
Brussels, Belgium

A. Pullman
Paris, France

P. Pyykkö
Turku, Finland

B. Roos
Lund, Sweden

K. Ruedenberg
Ames, IA

H. F. Schaefer III
Berkeley, CA

K. Schwarz
Vienna, Austria

I. Shavitt
Columbus, OH

M. Simonetta
Milan, Italy

A. C. Tang
Changchun, China

H. Taylor
Los Angeles, CA

P. Van Leuven
Antwerp, Belgium

A. Veillard
Strasbourg, France

M. Zerner
Guelph, Canada

The *International Journal of Quantum Chemistry* (ISSN 0020-7608) is published monthly in six issues per volume plus symposia by John Wiley & Sons, Inc. Copyright © 1982 by John Wiley & Sons, Inc., 605 Third Avenue, New York, New York 10158. All rights reserved. Reproduction or translation of any part of this work beyond that permitted by Sections 107 or 108 of the United States Copyright Law without the permission of the copyright owner is unlawful. Second-class postage paid at New York, New York, and at additional mailing offices.

The code and the copyright notice appearing at the bottom of the first page of an article in this journal indicate the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients, on the condition that the copier pay for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. The per-copy fee for each article appears after the dollar sign and is to be paid through the Copyright Clearance Center, Inc., 21 Congress St., Salem, MA 01970. (The fee for articles published prior to 1978 is $1.00 per article.) This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective work, or for resale. Such permission requests and other permission inquiries should be addressed to the publisher.

Subscription price: $450.00 per year. Postage and handling outside U.S.A.: $38.00 by surface; $130.00 by air. Allow four weeks to process a change of address. Back numbers, microfilm, and microfiche are available for previous years. Request price list from publisher.

Postmaster: Send address changes to Subscription Department, John Wiley & Sons, Inc., 605 Third Avenue, New York, New York 10158.

Claims for undelivered copies must be made no later than three months following the month of publication. Missing copies will be supplied when losses have been sustained in transit and where reserve stock will permit.

Manuscripts should be submitted in triplicate to Professor P.-O. Löwdin, Quantum Chemistry Group, University of Uppsala, Box 518, S-75120, Uppsala 1, Sweden. All other correspondence should be addressed to the Journals Department, John Wiley & Sons, Inc., 605 Third Avenue, New York, New York 10158, U.S.A.

International Journal of
QUANTUM CHEMISTRY

Contents for Volume XXI, 1982, Nos. 1–6

Issue No. 1, January 1982

**Proceedings of the
International Workshop on
Perturbation Theory at Large Order
(March 1981)**

Introduction
P. O. Löwdin and Y. Öhrn 1

Large Orders and Summability of Eigenvalue Perturbation Theory: A Mathematical Overview
B. Simon 3

Large Order Perturbation Theory in the Context of Atomic and Molecular Physics—Interdisciplinary Aspects
J. Čížek and E. R. Vrscay 27

Partitioning Technique, Perturbation Theory, and Rational Approximations
P.-O. Löwdin 69

Perturbation Theory in Large Order for Some Elementary Systems
C. M. Bender 93

Large-Order Perturbation Theory
T. T. Wu 105

Bender–Wu Formulas and Classical Trajectories: Higher Dimensions and Degeneracies
J. E. Avron 119

Unified Derivation of the Perturbation Series for the Real and Imaginary Parts of the Energy of Hydrogen in the Stark Effect and of the Negatively Anharmonic Oscillator
H. J. Silverstone 125

Padé Summations for the Real and Imaginary Parts of Atomic Stark Eigenvalues
W. P. Reinhardt 133

Numerical Estimates of the Convergence of the Rayleigh–Schrodinger Perturbation Expansions for the Energy Levels of Various Models of the Benzene Molecule
A. Pellegatti, J. Čížek, and J. Paldus 147

Representation Theory of $so(4,2)$ for the Perturbation Treatment Hydrogenic-Type Hamiltonians by Algebraic Method
B. G. Adams, J. Čížek, and J. Paldus 15

Failure of Strong Asymptotic Conditions in Four-Dimensional Field Theories
N. N. Khuri 173

Perturbation Theory via the Ricatti Equation
C. K. Au 179

Double Wells
R. Damburg and R. Propin 191

Meaning of the Perturbation Theory for a Class of Multiple-Well Anharmonic Oscillators
S. Graffi 195

Estimating Tunneling Phenomena
E. M. Harrell II 199

List of Participants 209

Proceedings of the Tarfala Workshop (August 1978)

Preface
P.-O. Löwdin, J.-L. Calais, and O. Goscinski 215

Relevance of the Techniques of Quantum Chemistry in Materials Science and Related Areas
M. R. Hayns 217

Is Quantum Chemistry Concerned with Materials Science?
J.-L. Calais 231

Towards a Molecular Theory of Phase Transitions in Fatty Acid Monolayers
L. J. Dunne and L. Combs 239

Converging SCF Calculations on Excited States
P. Corrêa De Mello, M. Hehenberger, and M. C. Zerner 251

Size Consistency Corrections for Configurations Interaction Calculations
E. J. Brändas, L. L. Combs and N. S. Correia 259

Some Properties of Reduced Density Matrices, Correlated and Uncorrelated, for Pure and Mixed States
O. Goscinski 269

On the Axioms of Quantum Theory Formulated as a Trace Algebra
P.-O. Löwdin 275

Information for Contributors 355

Issue No. 2, February 1982

Editorial: Density Functional Theory
P.-O. Lowdin, J.-L. Calais, and O. Goscinski 357

Electronic Structure of Beryllium
J. Oriade 359

Superoperator Approach to Propagator Approximations
B. Weiner and O. Goscinski 369

Variational-Perturbation Theory in the LCAO-MO Method for Closed-Shell Molecules
Yu. B. Malykhanov 399

Symmetry Groups of Chemical Graphs
K. Balasubramanian 411

Momentum Space Properties of Various Orbital Basis Sets Used in Quantum Chemical Calculations
A. M. Simas, A. J. Thakkar, and V. H. Smith, Jr. 419

Ab initio Calculations of the Electronic Structures of Dimethylnitrosamine (DMN) and Its Metabolite Hydroxydimethylnitrosamine (HDMN): A Possible Intermediate in Carcinogenesis by DMN
A. Skancke and C. Thomson 431

Structural Factors Affecting Aryl Hydrocarbon Hydroxylase Induction by Dibenzo-*p*-dioxins and Dibenzofurans
B. V. Cheney 445

Configuration Interaction Calculations of the Valence and the Inner Valence Levels of the CS Molecule
J. Müller 465

Small-Angle Electron Scattering and Electron Density in Carbon Dioxide
Y. Sasaki, S. Konaka, T. Iijima, and M. Kimura 475

Coupling of Internal Rotations in Propanelike Molecules
G. Wesenberg and F. Weinhold 487

Letter to the Editor

In Defense of the Hohenberg–Kohn Theorem and Density Functional Theory
M. Levy and J. P. Perdew 511

Issue No. 3, March 1982

Transferable Integrals in a Deformation Density Approach to Crystal Calculations. I. Crystal Harmonics and Their Properties
J. Avery, P.-J. Ørmen, and I. Chatterjee 515

Note on Calculations by Hypervirial Relations and Sufficient Conditions for These Relations: Box Potential and Harmonic Oscillator Models
T. Terasaka and K. Sakamoto 543

An initio Hartree–Fock–Slater Calculation of Tetrathiafulvalene (TTF) and the TTF^{1+} and TTF^{2+} Ions.
M. Trsic and W. G. Laidlaw 557

Stability and Bonding of Disilyne and Its Isomers: A Generalized Valence Bond-Effective Potential Study
L. C. Snyder, Z. R. Wasserman, and J. W. Moskowitz 565

Spectra of Chemical Trees
K. Balasubramanian 581

General Linear Group Approach to Bivariational Problems
B. Weiner 591

Variational Solutions of a First-Order Perturbation Equation
H. Hamano 611

Connections between Perturbation Theory and the Van Vleck Transformation: Illustrative Calculation on the Perturbed Harmonic Oscillator
P. Westhaus 617

Construction of an Effective Hamiltonian for Open-Shell Molecular Systems
S. Biskupič and V. Kvasnička 633

Symmetry Properties of Chemical Graphs. IV. Rearrangement of Tetragonal–Pyramidal Complexes
M. Randić and V. Katović 647

CNDO/2 and INDO Studies of Structure and Relative Stability of a Series of H*AB*-H*BA* Systems of Mixed First- and Second-Row Composition
B. R. De, S. Bhattacharjee, and A. B. Sannigrahi 665

Letter to the Editor

Trivial Off-Diagonal Hellmann–Feynman Formulas
F. M. Fernández and E. A. Castro 671

Issue No. 4, April 1982

Hypervirial Extension for Energies of Parameter-Dependent Systems
F. M. Fernández and E. A. Castro 673

Change Transfer and Induced Polarization in Model Peptide–Ion Complexes
P. G. Mezey, G. Del Re, P. Otto, S. Suhai, and J. Ladik 677

Uniform Quality Gaussian Basis Sets for Molecular Calculations. V. Property Optimization: A Study on H_2O
R. Daudel, R. A. Poirier, and I. G. Csizmadia 699

Calculation of Periodic Molecular Systems with Perturbed Periodicity within the PCILO Framework. I. Method
R. Lochmann and Th. Weller 711

Periodic Table of the Elements and the Thomas–Fermi Atom
H. Essén 717

Complex Coordinate Rotation Calculation of Branching Ratios
Z. Bačić and J. Simons 727

Virial Theorem and Boundary Conditions for Approximate Wave Functions
F. M. Fernández and E. A. Castro 741

Calculation in k Space of Integrals Arising in the Theory of van der Waals Forces
P. Malinowski, A. C. Tanner, K. F. Lee, and B. Linder 753

Announcement 767

Information for Contributors 769

Issue No. 5, May 1982

Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. I. Simple Catacondensed Systems
S. El-Basil 771

Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. II. Benzenoid Systems Having Four to Seven Fused Benzene Rings: "Pseudodegenerate" States
S. El-Basil 779

Novel Graph-Theoretical Approach to Estimating the Relative Importance of Individual Kekulé Valence Structures. III. Nonalternate and Nonbenzenoid Hydrocarbons
S. El-Basil 793

Ab initio Calculations of Sulfur-Containing Compounds. I. Uniform Quality Basis Sets for Sulfur: Total Energies and Geometries of H_2S
R: A. Poirier, R. Daudel, P. G. Mezey, and I. G. Csizmadia 799

CNDO/2 Calculations of Relaxation and Reconstruction of Diamond and Silicon[111] Surfaces
I. László 813

Diagram Approach to Group Algebraic Methods
R. J. Black and G. E. Stedman 823

Critical Examination of Approximate LCAO MO Methods. I. Reasons for the Failure of the CNDO and INDO Methods in Theoretical Conformational Analysis of Conjugated Compounds
P. Birner and H.-J. Hofmann 833

Calculation of Relaxed Orbital Binding Energies in Atoms: Zinc and Cadmium
M. P. Das 845

Semiempirical Molecular Orbital Calculations on Octahedral Aquo Complexes of Transition Metal Ions: σ-Donor Ability of Water
S. P. Bhattacharyya 851

Feenberg Scaling and Higher-Order Invariants in Rayleigh–Schrödinger Perturbation Theory
K. Bhattacharyya 857

Charge and Spin Correlation Structures of Conjugated π Systems: Analysis of Full CI Wave Functions of the PPP Hamiltonian
K. Hashimoto 861

Hypervirial Analysis of Enclosed Quantum Mechanical Systems. IV. Further Comments
F. M. Fernández and E. A. Castro 875

Reduced Local Energy as a Criterion for the Accuracy of Approximate Hartree–Fock Wave Functions. Application to H_2O and CH_4
H. H. Grelland and J. Almlöf 885

Theory of the Electron Distribution in Compressed Atoms at High Temperatures
P. Csavinszky 899

Scaled One-Electron Hamiltonian Model for Open-Shell LCAO–MO–SCF Calculations: Comparison with the Restructed Open-Shell Method of Roothaan
M. Banerjee and S. P. Bhattacharyya 905

Cluster CPA Calculations for Infinite and Half-Infinite Chains and Applications to Coupled Polymer Chains
R. S. Day and J. Ladik 917

Virial Fragments and the Hohenberg–Kohn Functional
E. B. Ludeña and V. Mujica 927

Letters to the Editor

Comment on Hypervirial Relations for Bounded Systems
R. J. Swenson 937

Simple Derivation of the Potential Energy Gradient for an Arbitrary Electronic Wave Function
T. U. Helgaker 939

Book Reviews

Understanding Physical Chemistry. By Arthur W. Adamson
Reviewed by Sten Lunell 941

Announcements 943

Issue No. 6, June 1982

Interpretation of the Antitumour Activity of Some Diacridines
P. G. Abdul-Ahad and G. A. Webb 945

Molecular Tight-Binding Method. I. Many-Electron Method for Hole Bands of Molecular Crystals
L. Z. Stolarczyk 967

Molecular Tight-Binding Method. II. One- and Many-Electron Method for Excess Electron Bands of Molecular Crystals
L. Z. Stolarczyk 993

Permutation-Group Classification and Description of the Feynman–Goldstone Diagrams
V. Kvasnička 1003

Particlelike Excitations in the Polypeptide Chain Model
V. K. Fedyanin and L. V. Yakushevich 1019

Molecular Orbital Study on the Active Center of Lactate Dehydrogenase
J. Krechl and J. Kuthan 1029

Variational Marginal Amplitudes
G. Hunter and C-C. Tai 1041

Some Remarks on the Use of Rational Functions as Variational Functions
P. Jolly, K. V. Sane, R. P. Saxena, and P. K. Srivastava 1051

Transformation of Spin Projected Slater Determinants under Orbital Permutation
G. A. Gallup 1057

Equation Matricielle de Hartree–Fock Permettant de Déterminer la $n^{\text{ième}}$ Harmonique
F. Smet and A. V. Groenendael 1061

Evaluation of Two-Center Overlap and Coulomb Integrals Derived from Slater-Type Orbitals
H. W. Jones 1079

Potential Adaption: Use of Polynomials as Anharmonic Oscillator Potentials
K. Gustav and R. Colditz 1091

Some Comments about Tensor Virial Theorem and Linear Transformations
F. M. Fernández and E. A. Castro 1097

Quantitative Structure Activity Relationships for Some Antitumor Platinum(II) Complexes
P. G. Abdul-Ahad and G. A. Webb 1105

Long-Range Interaction Coefficients between H, He^+, He, and Li^+
S. I. Easa and F. N. Yousif 1117

Letter to the Editor

Matrix Analysis of N-Representability Necessary Conditions
E. S. Kryachko 1123

Author Index to Volume XXI 1127

Information for Contributors 1131

Volume Title Page i

Volume Contents iii